LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039088.D
Acq On : 22 Mar 2023 12:18
Operator : CG/JU
Sample : 01978-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20230316

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	295	301	308	rBV	1806699	2441495	12.25%	2.341%
2	5.522	373	380	389	rBV	2957674	4141608	20.79%	3.971%
3	7.128	645	653	661	rBV	1600370	2430668	12.20%	2.331%
4	7.963	789	795	803	rBV	1091385	1735488	8.71%	1.664%
5	9.134	986	994	1002	rBV	4004647	6655218	33.40%	6.382%
6	10.780	1266	1274	1282	rBV	1392479	2335285	11.72%	2.239%
7	13.233	1684	1691	1709	rVB	9953833	14254363	71.54%	13.669%
8	14.604	1918	1924	1934	rBV	1948911	2923559	14.67%	2.803%
9	15.015	1989	1994	2006	rVB	160035	280499	1.41%	0.269%
10	15.163	2014	2019	2027	rVB	117656	211372	1.06%	0.203%
11	15.957	2145	2154	2160	rBV4	170854	362134	1.82%	0.347%
12	16.092	2171	2177	2188	rBV	7204907	10209041	51.24%	9.789%
13	16.380	2220	2226	2236	rVB2	415342	724322	3.64%	0.695%
14	16.733	2280	2286	2297	rVB3	591846	1205976	6.05%	1.156%
15	16.892	2309	2313	2320	rBV	166651	227415	1.14%	0.218%
16	17.351	2385	2391	2396	rBV	2444610	3374042	16.93%	3.235%
17	18.015	2499	2504	2516	rVB2	938327	1418720	7.12%	1.360%
18	18.251	2534	2544	2552	rBV	5861501	9090862	45.63%	8.717%
19	18.315	2553	2555	2564	rVB	323883	454502	2.28%	0.436%
20	18.521	2585	2590	2594	rBV	1824154	2731888	13.71%	2.620%
21	18.568	2594	2598	2612	rVB	2122106	3346937	16.80%	3.209%
22	19.374	2731	2735	2737	rBV	238166	326522	1.64%	0.313%
23	19.398	2737	2739	2748	rVB3	213191	360210	1.81%	0.345%
24	19.521	2754	2760	2782	rVB	3427347	5083634	25.51%	4.875%
25	19.974	2831	2837	2842	rBV	15867541	19925132	100.00%	19.106%
26	21.233	3048	3051	3059	rBV2	223683	257508	1.29%	0.247%
27	21.527	3097	3101	3108	rBV	2840041	3666906	18.40%	3.516%
28	23.962	3509	3515	3525	rVB2	2137717	4110594	20.63%	3.942%

Sum of corrected areas: 104285900

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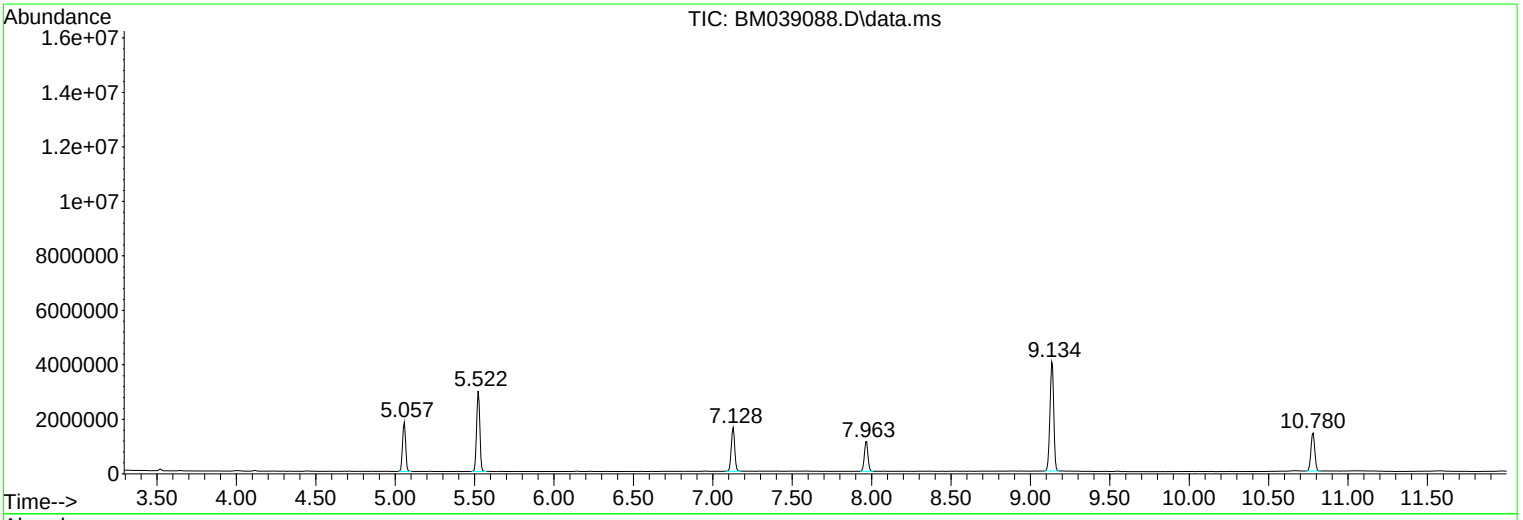
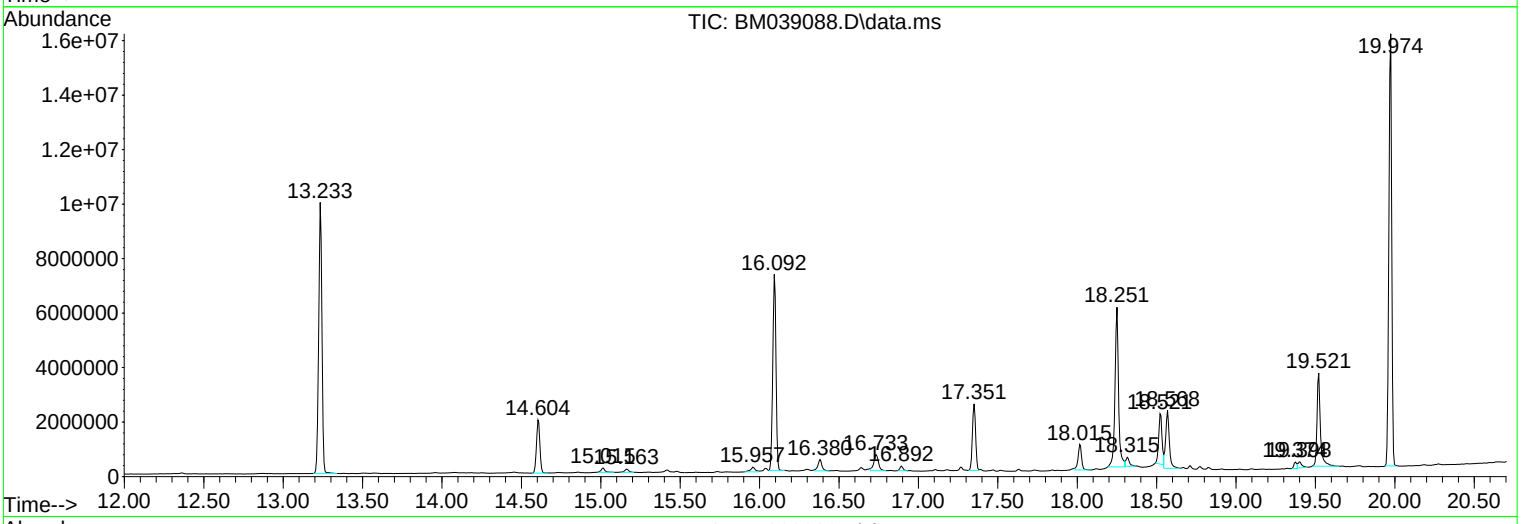
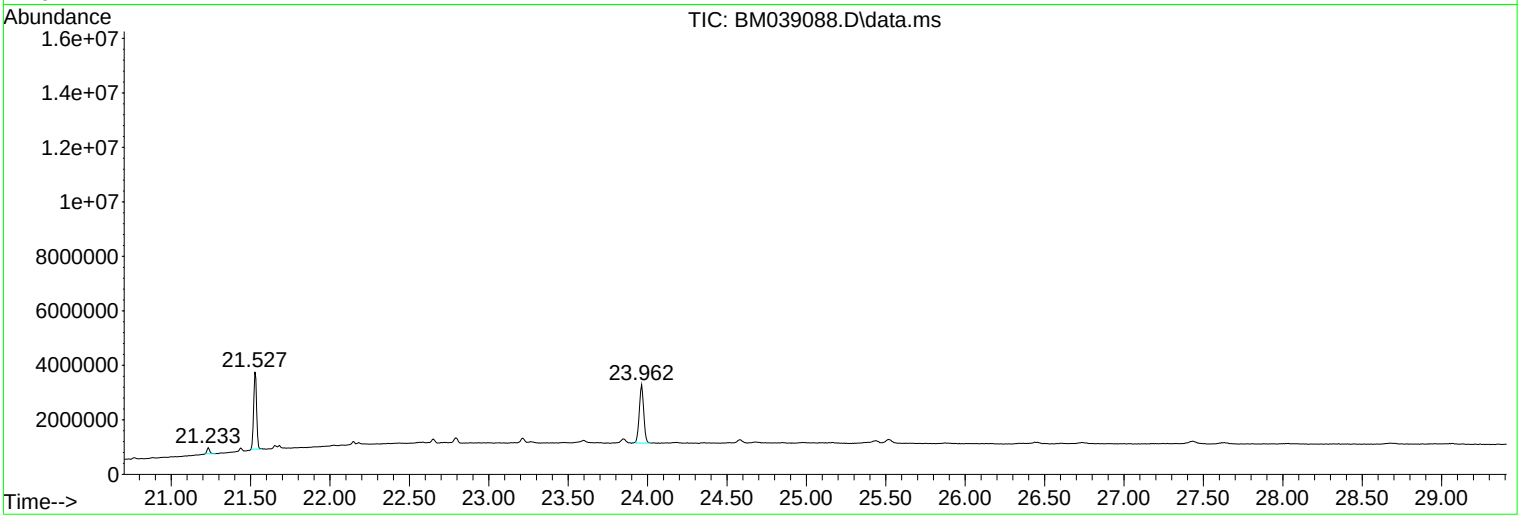
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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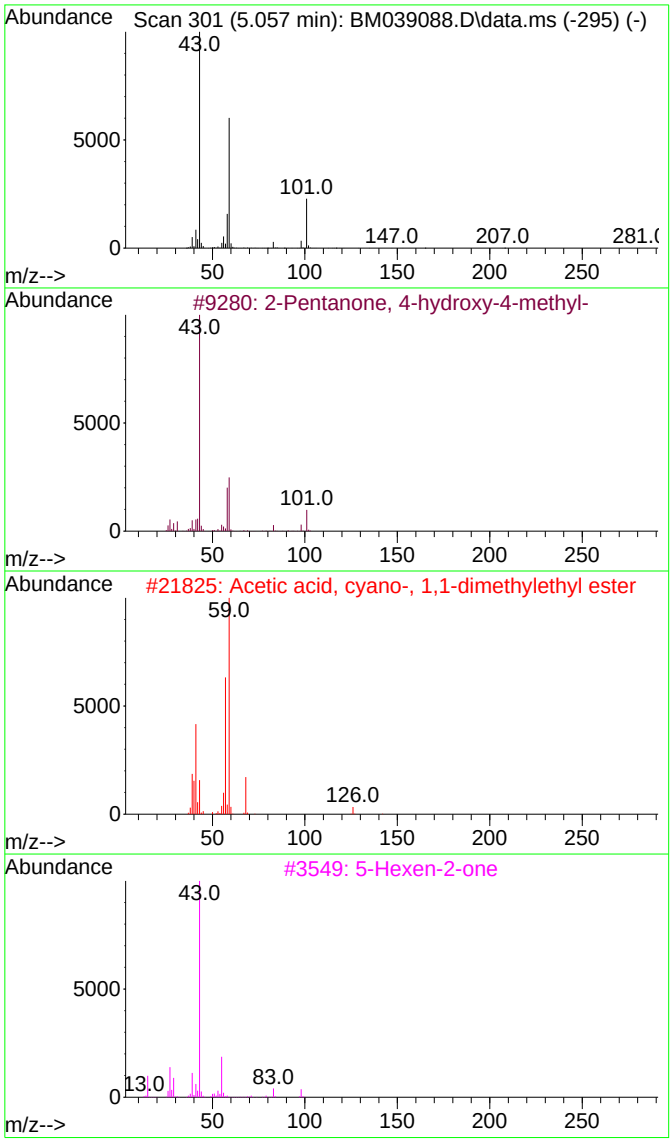
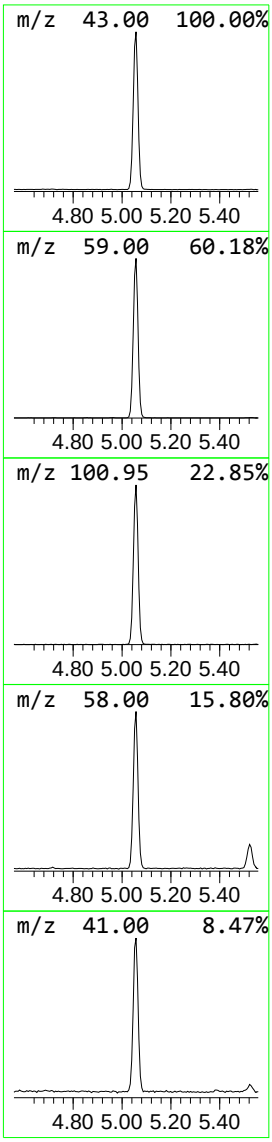
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	28.14 ng	2441500	1,4-Dichlorobenzene-d4	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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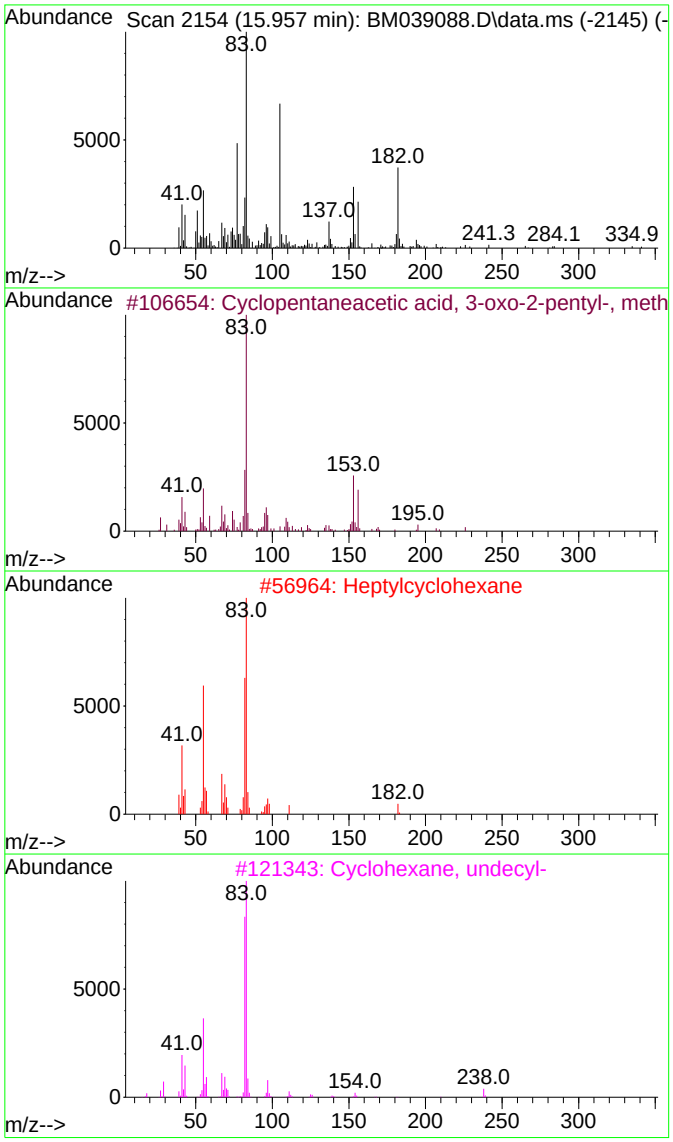
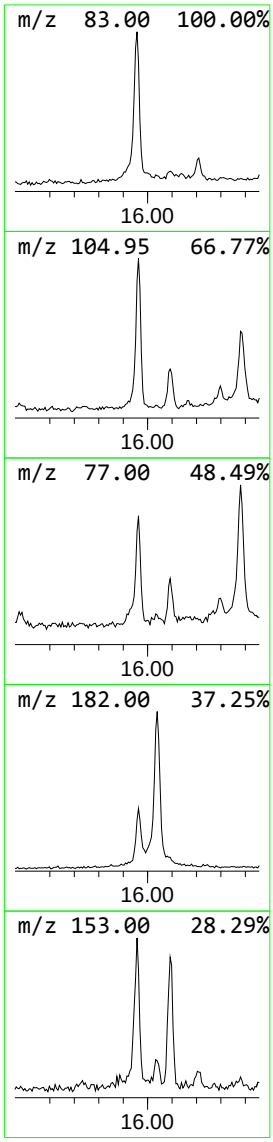
****
Peak Number 2 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.48 ng	362134	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	83
2	Heptylcyclohexane	182	C13H26	005617-41-4	45
3	Cyclohexane, undecyl-	238	C17H34	054105-66-7	27
4	Glycine, N-(2-methyl-1-oxo-2-but...	171	C8H13NO3	055649-53-1	27
5	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	27





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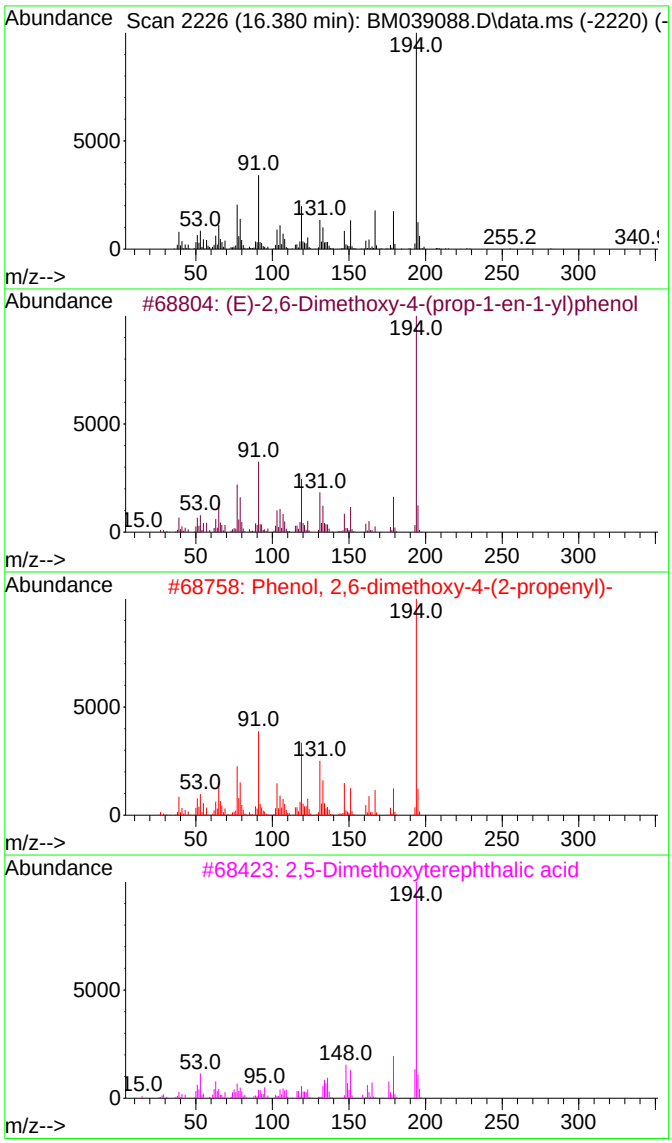
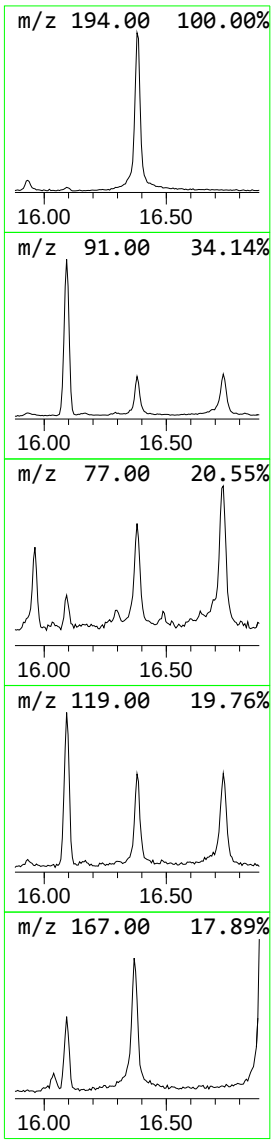
****
Peak Number 3 (E)-2,6-Dimethoxy-4-(prop-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.380	4.29 ng	724322	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-2,6-Dimethoxy-4-(prop-1-en-1...	194	C11H14O3	020675-95-0	98
2	Phenol, 2,6-dimethoxy-4-(2-prope...	194	C11H14O3	006627-88-9	93
3	2,5-Dimethoxyterephthalic acid	194	C10H10O4	007310-97-6	50
4	2-Hydroxy-4-isopropyl-7-methoxyt...	194	C11H14O3	089647-85-8	50
5	2,5-cyclohexadiene-1,4-dione, 2,...	194	C10H14N2O2	1000400-30-4	47





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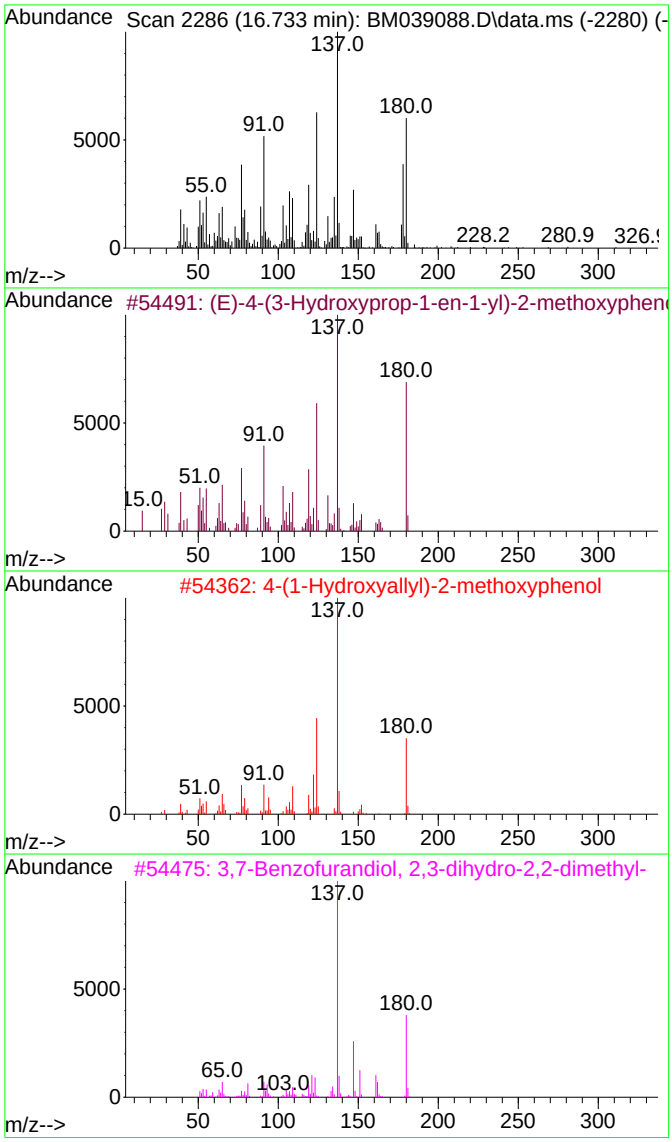
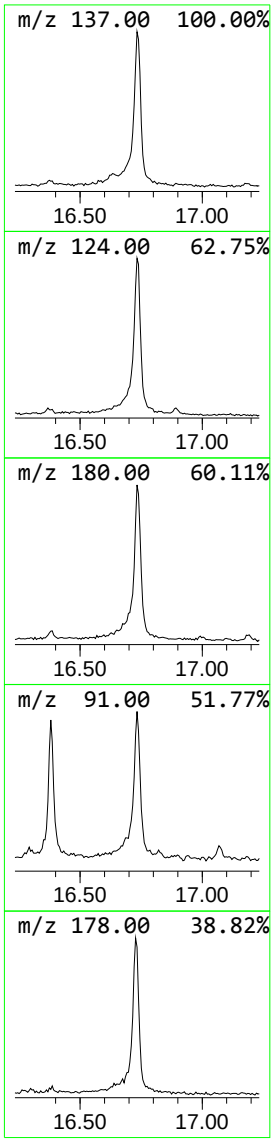
****

Peak Number 4 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	7.15 ng	1205980	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	86
2	4-(1-Hydroxyallyl)-2-methoxyphenol	180	C10H12O3	112465-50-6	53
3	3,7-Benzofurandiol, 2,3-dihydro-...	180	C10H12O3	017781-15-6	41
4	1-(Prop-2-ynyloxy)-3,4-methylene...	178	C10H10O3	019202-22-3	30
5	2-Methylnicotinic acid	137	C7H7NO2	003222-56-8	20





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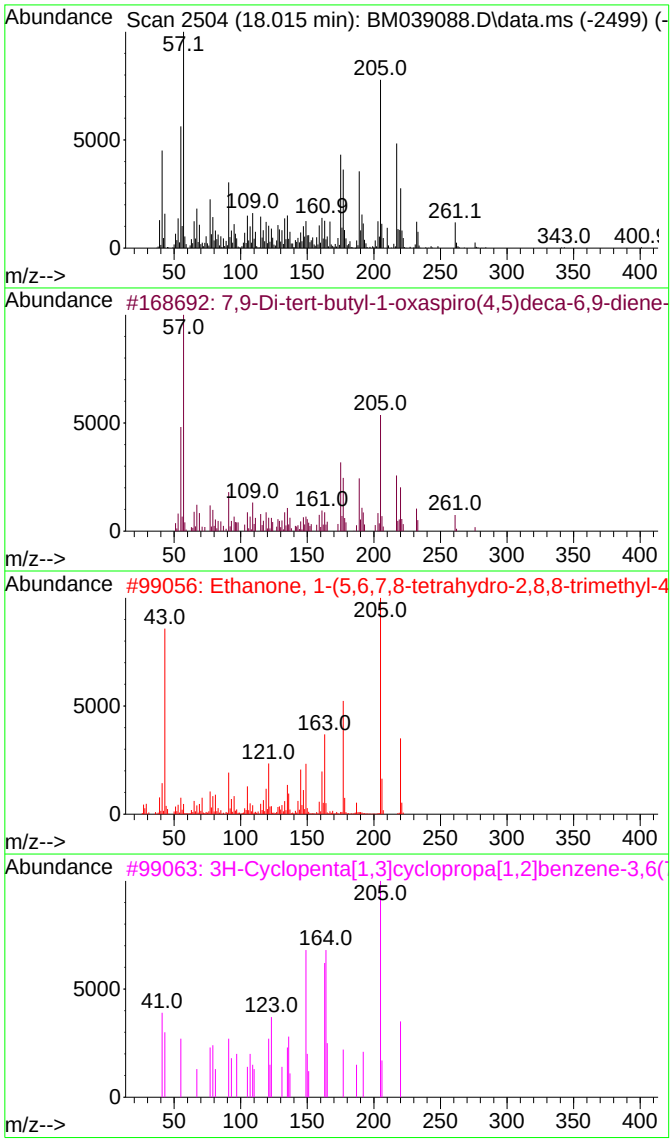
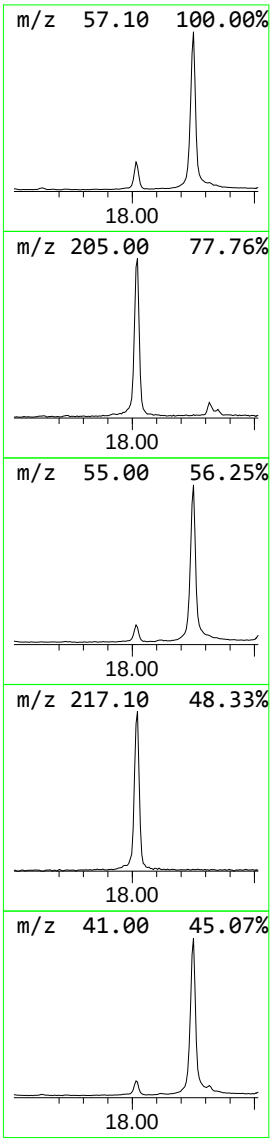
****
Peak Number 5 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.015	8.41 ng	1418720	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
3	3H-Cyclopenta[1,3]cyclopropa[1,2...	220	C14H20O2	066708-18-7	46
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	41
5	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	38





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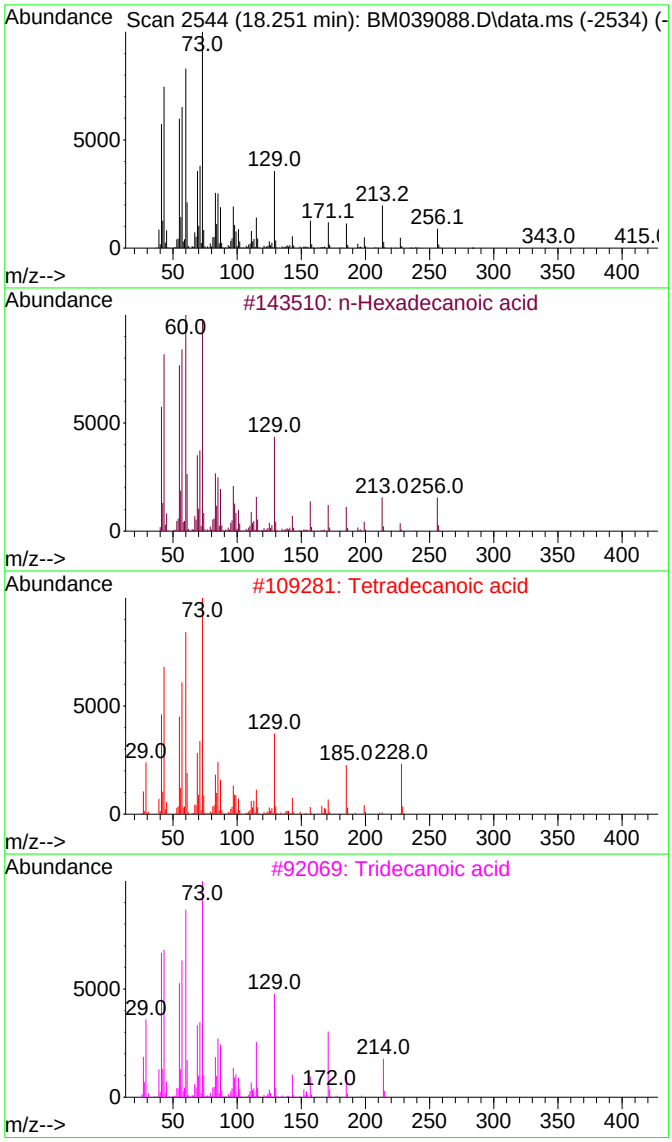
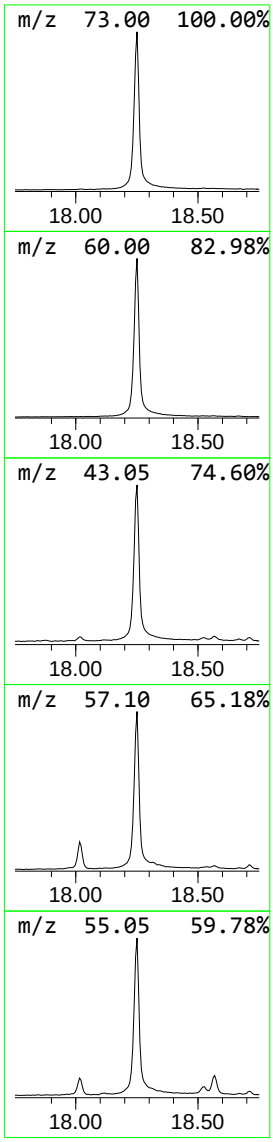
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.251	53.89 ng	9090860	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





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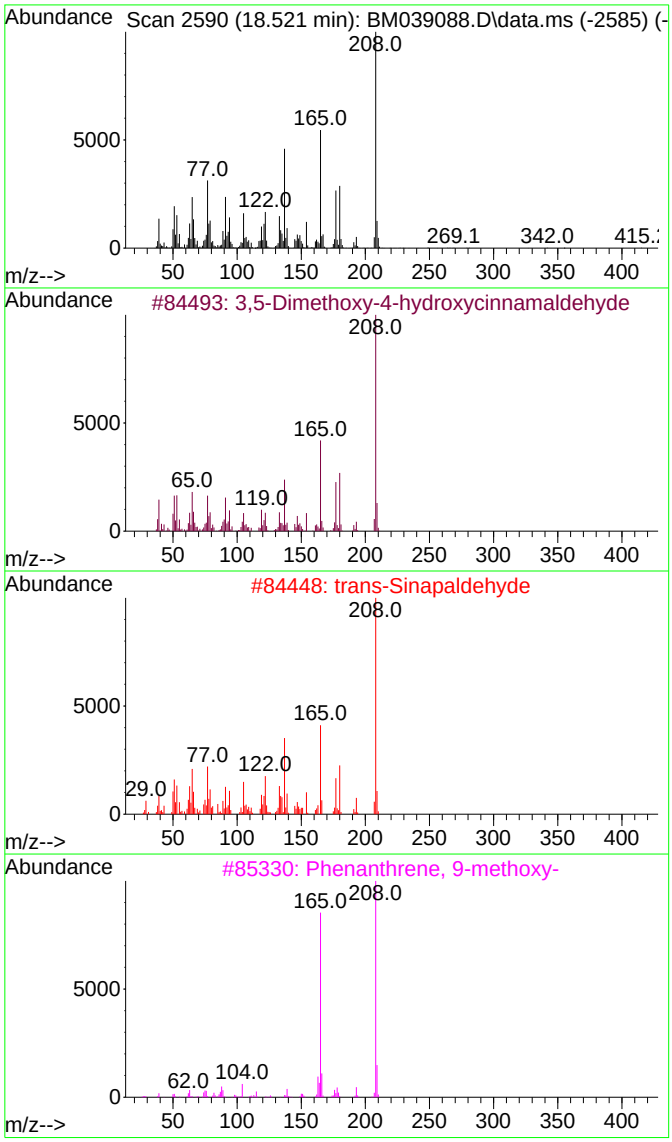
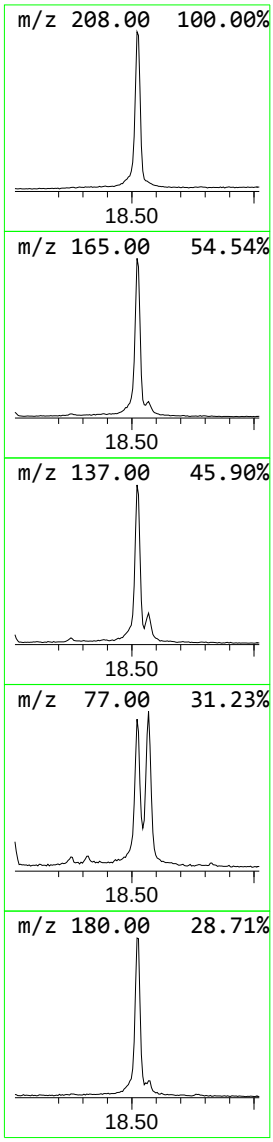
****

Peak Number 7 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.521	16.19 ng	2731890	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	97
2	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	89
3	Phenanthrene, 9-methoxy-	208	C15H12O	005085-74-5	46
4	4-(4-Fluoro-3-methylphenyl)-1,3-...	208	C10H9FN2S	003830-48-6	45
5	2-Propenoic acid, 3-(2,4-dimetho...	208	C11H12O4	016909-09-4	43





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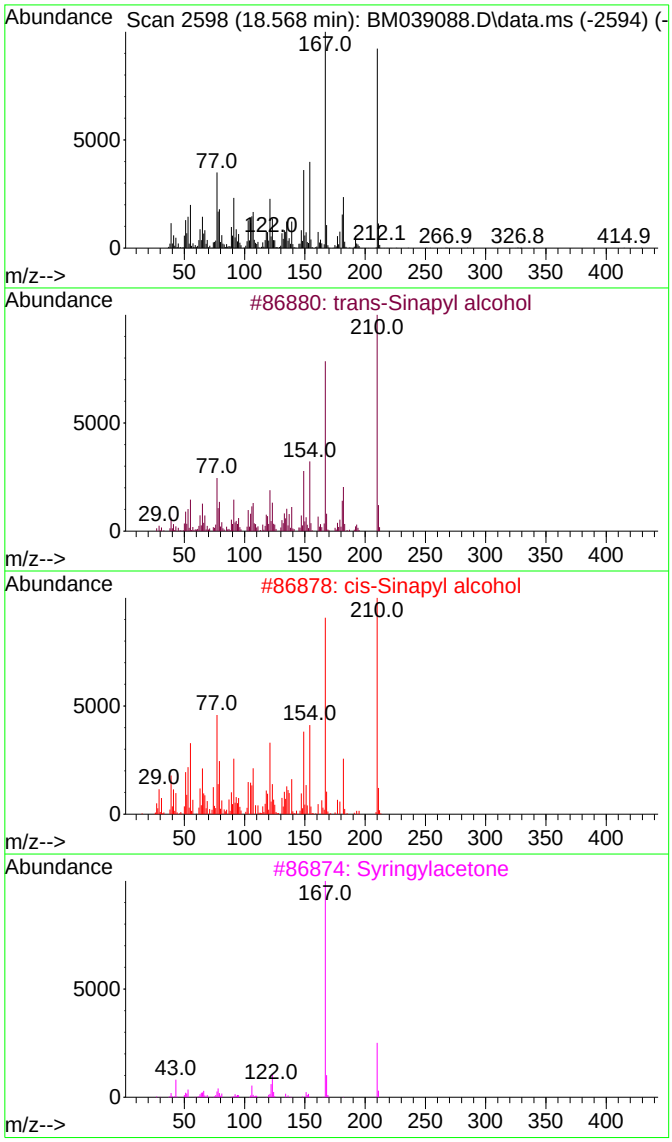
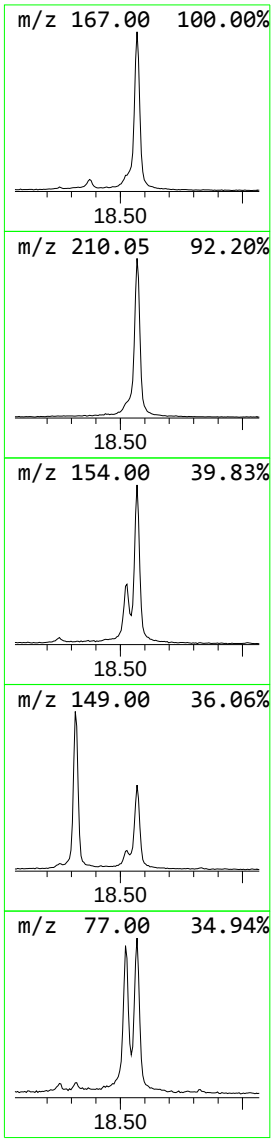
****

Peak Number 8 trans-Sinapyl alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.568	19.84 ng	3346940	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	98
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	96
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	55
5	2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	52





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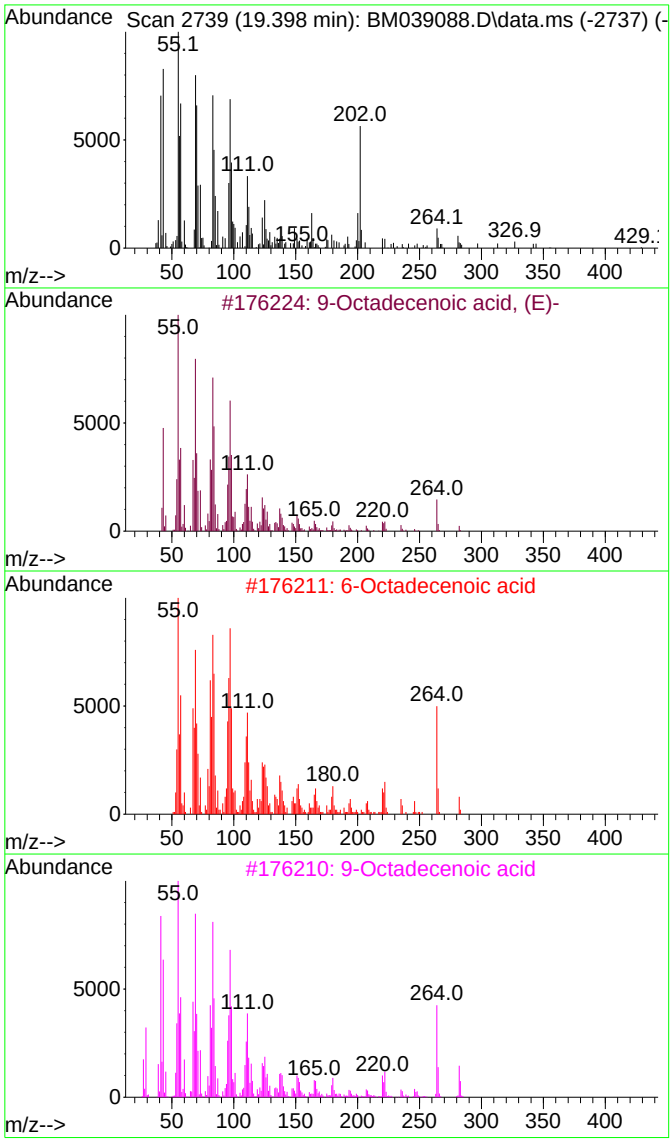
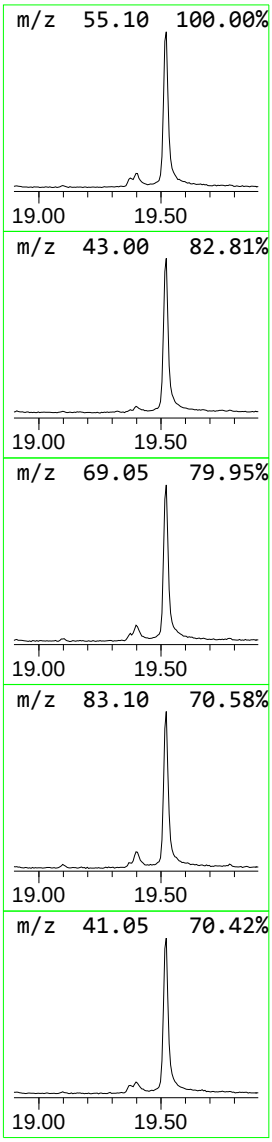
****

Peak Number 9 9-Octadecenoic acid, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	2.14 ng	360210	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	93
2	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	90
3	9-Octadecenoic acid	282	C18H34O2	002027-47-6	86
4	Oleic Acid	282	C18H34O2	000112-80-1	76
5	Carbonic acid, dodecyl 2,2,2-tri...	360	C15H27Cl3O3	1000314-55-8	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039088.D
Acq On : 22 Mar 2023 12:18
Operator : CG/JU
Sample : 01978-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20230316

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

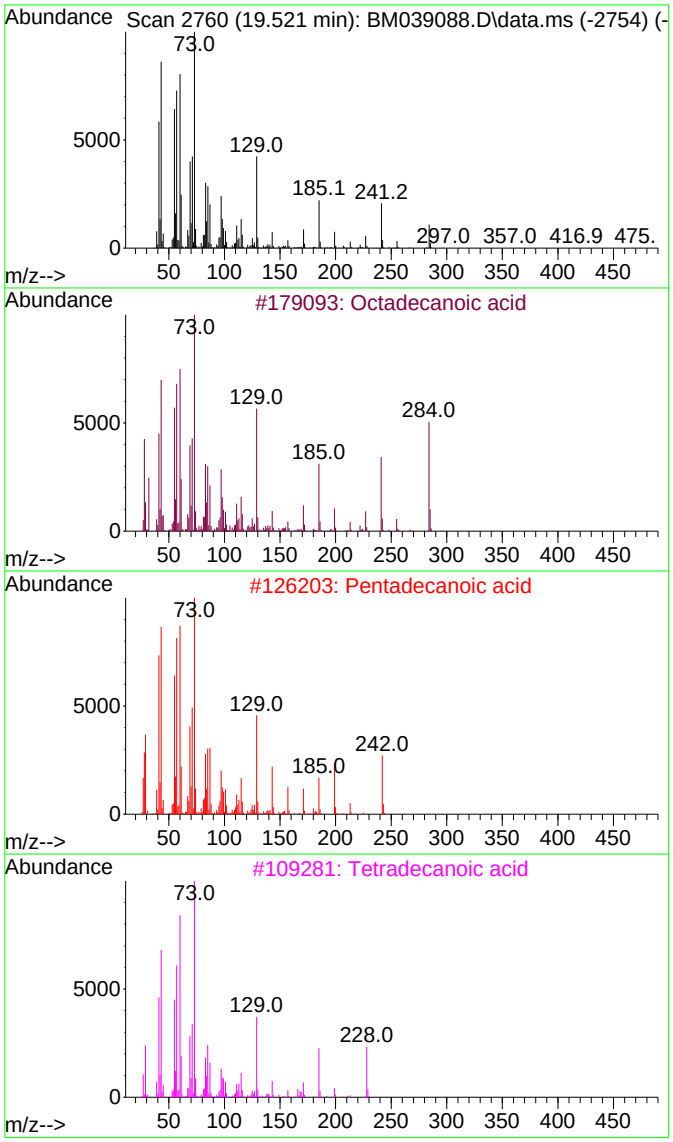
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

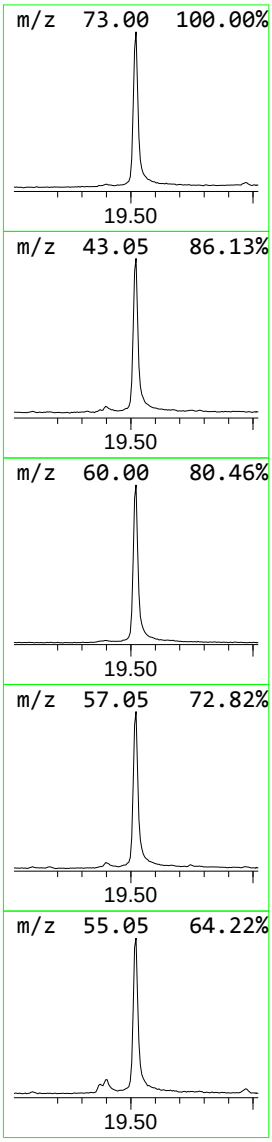
****

Peak Number 10 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.521	27.73 ng	5083630	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039088.D
Acq On : 22 Mar 2023 12:18
Operator : CG/JU
Sample : 01978-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20230316

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	28.1	ng	2441500	1	7.969	1735490	20.0
Cyclopentaneace...	15.957	2.5	ng	362134	3	14.604	2923560	20.0
(E)-2,6-Dimetho...	16.380	4.3	ng	724322	4	17.351	3374040	20.0
(E)-4-(3-Hydrox...	16.733	7.2	ng	1205980	4	17.351	3374040	20.0
7,9-Di-tert-but...	18.015	8.4	ng	1418720	4	17.351	3374040	20.0
n-Hexadecanoic ...	18.251	53.9	ng	9090860	4	17.351	3374040	20.0
3,5-Dimethoxy-4...	18.521	16.2	ng	2731890	4	17.351	3374040	20.0
trans-Sinapyl a...	18.568	19.8	ng	3346940	4	17.351	3374040	20.0
9-Octadecenoic ...	19.398	2.1	ng	360210	4	17.351	3374040	20.0
Octadecanoic acid	19.521	27.7	ng	5083630	5	21.527	3666910	20.0